OPTIMAL SYMMETRICAL DESIGNS

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CHAPTER I

INTRODUCTION

1.1 Description of the Problem

The P^n factorial has been widely used in industrial, educational, and agricultural applications in recent years. Although articles appear frequently in the literature which investigate different aspects of factorial designs, one problem of importance which deserves further investigation is that of determining optimal designs based on special criteria. Another aspect of factorial designs is that of fractions of factorials. These are very useful when the number of factors, n, or the number of levels, P, become large.

This investigation is concerned with developing symmetrical designs which are fractions of factorials based on the expansion of P^n as $(\sum_{i=1}^{k} p_i)^n$. Chapters II and III are devoted to this development. Different symmetrical designs for a given number, N, of design points are compared using five optimality criteria and assuming the two-dimensional, quadratic model

$$y(x_1, x_2) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1^2 + \beta_4 x_1 x_2 + \beta_5 x_2^2 + \epsilon$$

where $\epsilon \sim N(0, \sigma^2)$. In Chapter IV, three of the optimality criteria, minimax variance of $\hat{\beta}_i$, minimum generalized variance of $\hat{\beta}$ and minimax characteristic root of $(X'X)^{-1}$, which is a minimax variance of uncorrelated linear functions of the $\hat{\beta}_i$'s, are studied. The average variance of the estimated response in the square region R and the circular region R_c is determined for any distribution of the probability mass to the region of interest. Chapter V deals with this problem and with the designs which have the minimum average variance of the estimated response.

These symmetrical designs were developed to be used in experiments which are of an investigative nature such as optimum seeking experiments or experiments used to determine the shape of a response surface in the region of a maximum response.

1.2 Review of the Literature

In the area of response relationships, a rather detailed review of the literature through 1958 has been presented by Folks (1), and from 1958 through 1963 has been presented by Gillett (3). Therefore a review of the literature which is pertinent to the development of this thesis will be presented here.

A number of articles have appeared recently which approach the optimal design problem from a probability standpoint. Such is the case in articles by Kiefer (4), (5), and Kiefer and Wolfowitz (6). The optimal designs which they obtained are only optimal to within a given approximation of the true theoretical optimal design. Folks (1) approaches the problem of determining optimal experimental designs for various criteria by considering two cases; namely, the case where the number of design points, N, is even and the case where N is odd. By this procedure, exact optimal designs were determined in the one-dimensional case for the following criteria:

(i) $\min_{x} \max_{u} \operatorname{var} \hat{y}(u)$

(ii) $\min_{x} \operatorname{ave}_{u} \operatorname{var} \hat{y}(u)$

(iii) $\min_{x} \operatorname{gen\ var} \hat{y}(u)$

where var $\hat{y}$ (u) is the variance of the estimated response at u. Also, exact optimal designs for bias and mean square error considerations in the one-dimensional case and for variance and bias considerations in the two-dimensional case were determined when the number of design points was a certain multiple of four.

Gillett (3) determined exact optimal designs for several polynomial models. From a restricted class of models, a model is selected as one which is optimal in the sense of minimizing some form of the bias. Also, the average variance of the estimated response is investigated for every distribution of the total mass to the region of interest assuming a linear model.

In recent years fractional factorials have received much attention. A new approach to factorial experimentation was suggested by Fry (2), developed by Williams (8), and extended by Thomas (7). Williams developed fractions obtained by considering the P^n factorial in an algebraic context as

$$P^n = (p_1 + p_2)^n = \sum_{i=0}^{n} \binom{n}{i} p_1^{n-i} \; p_2^{i}$$

where $p_1 + p_2 = P$ and p_1 and p_2 are positive integers. The new fractions are then obtained by expanding $(p_1 + p_2)^n$ as a binomial. Thomas (7) extended this concept to the case

$$\begin{aligned} P^n &= (\sum_{i=1}^{k} p_i)^n \\ &= \sum_{n_1=0}^{n} \sum_{n_2=0}^{n} \cdots \sum_{n_k=0}^{n} [n!/(n_1!n_2! \ldots n_k!)] \; p_1^{n_1} \; p_2^{n_2} \ldots p_k^{n_k} \end{aligned}$$

where $\sum_{i=1}^{k} n_i = n$, $\sum_{i=1}^{k} p_i = P$ and $p_1, p_2, \ldots, p_k$ are positive integers.

A relationship will be established now in the following chapter between these concepts and symmetrical designs.

CHAPTER II

SYMMETRY AND OPTIMALITY CRITERIA

2.1 Models to be Used

The design points Z_i are the points in an n-dimensional space where the observations are to be taken. The n-dimensional space consisting of all design points will be called the factor space. An experimental design will be defined as a procedure which indicates where the design points are to be located and how many observations are to be taken at each design point. It is always possible to code the levels of the factor space into the coded factor space where the points will be denoted by $X^* = (x_1, x_2, \ldots, x_n)$, $-1 \leq x_i \leq 1$. Each x_i represents the coded levels of factor i. Henceforth we shall assume that the levels are equally spaced in the region of experimentation and when we use the words, design points, we shall mean the coded design points, X^*.

In this thesis we shall consider primarily two-dimensional models where the response will be given by the quadratic model

$$y(x_1, x_2) = \beta_0 x_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1^2 + \beta_4 x_1 x_2 + \beta_5 x_2^2 + \epsilon$$

where $-1 \leq x_i \leq 1$, $i = 1,2$, $x_0 = 1$, and $\epsilon \sim \text{NID}(0, \sigma^2)$.

All of the observations assuming a given model may be represented in matrix form as $Y = X\beta + \epsilon$, where β is a vector consisting of a function of the β_i's and X is the design matrix for N coded design points. For the two-dimensional quadratic model, X is given as

$$X = \begin{bmatrix} 1 & x_{11} & x_{21} & x_{11}^2 & x_{11}x_{21} & x_{21}^2 \\ 1 & x_{12} & x_{22} & x_{12}^2 & x_{12}x_{22} & x_{22}^2 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 1 & x_{1N} & x_{2N} & x_{1N}^2 & x_{1N}x_{2N} & x_{2N}^2 \end{bmatrix}$$

where each observation $y_i(x_1, x_2)$, $i = 1, \ldots, N$ has associated with it a vector representing the independent variables denoted by (x_{1i}, x_{2i}).

Let u be a variable point in the two-dimensional factor space and let U represent the row of the design matrix which corresponds to the point u. The response at any point u in the factor space is estimated by

$$\hat{y}(u) = U\hat{\beta} = U(X'X)^{-1}\,X'Y$$

where $\hat{\beta}$ is the least squares and maximum likelihood estimate of β.

The variance of the estimated response, denoted by var $\hat{y}(u)$, is given by

$$\text{var}\ \hat{y}(u) = U(X'X)^{-1}\,U'\sigma^2$$

In this thesis σ^2 will be considered equal to unity unless otherwise specified.

2.2 Definition of Symmetry

In this thesis we shall be concerned only with fractions of a P^n factorial. These fractions will possess a special property called "symmetry". They will be symmetrical in the sense that all design points will be taken symmetrically, using the rule defined below for symmetry, with respect to the center of the region $-1 \leq x_i \leq 1$, $i = 1,2,\ldots,n$.

For the two-dimensional case we shall denote (x_{1i}, x_{2j}) by $[i, j]$ where $i, j = 1,2,\ldots, P$ represent the P levels of the factors x_1 and x_2. By "ϵD" we shall mean "belong to the design D" where D denotes a symmetrical design. Then symmetry will be defined as follows:

Rule for Symmetry:

(1) If $i = j$, then $[i, j] \epsilon D$ implies that $[P - i + 1, P - j + 1]$, $[P - i + 1, j]$ and $[i, P - j + 1]$ also ϵD.

(2) If $i \neq j$, then $[i, j] \epsilon D$ implies that $[P - i + 1, P - j + 1]$ $[P - i + 1, j]$, $[i, P - j + 1]$, $[j, i]$, $[P - j + 1, P - i + 1]$ $[j, P - i + 1]$ and $[P - j + 1, i]$ also ϵD.

The "rule for symmetry" is derived from the expansion of $(\sum_{i=1}^{k} p_i)^2$ which will be discussed below.

Using the rule for symmetry, all points in a P^2 are partitioned into one, four or eight point groups. If P is odd, the one-point group is the center point; if P is even, there is no one-point group.

Each of these symmetrical groups (fractions) may be obtained by expressing P^n as $(\sum_{i=1}^{k} p_i)^n$, a method developed by Thomas (7), which we need now. Thus P^n may be written as

$$P^n = (\sum_{i=1}^{k} p_i)^n = \sum_{n_1=0}^{n} \sum_{n_2=0}^{n} \cdots \sum_{n_k=0}^{n} [n!/(n_1!n_2! \ldots n_k!)] p_1^{n_1} p_2^{n_2} \cdots p_k^{n_k}$$

where $\Sigma n_i = n$, $p_1 + p_2 + \ldots + p_k = P$ and $p_1, \ldots, p_k$ are positive integers. If we consider each term in the expansion of the multinomial, we have a factorial arrangement of treatments multiplied by the coefficient $n!/(n_1!n_2! \ldots n_k!)$. The multinomial coefficient of each term gives the number of balanced factorials of each type. The number of reduced symmetrical designs for a specified P^n and N may be obtained from the expression $\sum_{n_1=0}^{n} \sum_{n_2=0}^{n} \ldots \sum_{n_k=0}^{n}$ (1) subject to $\Sigma n_i = n$.

Example 1.1: Consider the expansion $P^2 = (p_1 + p_2 + p_3)^2 = p_1^2 + p_2^2 + p_3^2 + 2p_1p_2 + 2p_1p_3 + 2p_2p_3$. This expansion contains 9 reduced factorials but there are only $\binom{3}{1} + \binom{3}{2} = 6$ reduced symmetrical designs where by "reduced" we mean that each design is not made up of two or more symmetrical groups. The terms in the expansion represent these 6 reduced symmetrical designs. For example, consider the expression $2p_1p_2$ in the above expansion. This represents one reduced symmetrical design in the expansion of P^2. The "2" in $2p_1p_2$ represents the different orders the p_i values may assume which are p_1xp_2 and p_2xp_1. If we represent the two factors by A and B, then factor A has p_1 levels in the p_1xp_2 factorial and p_2 levels in the p_2xp_1 factorial and factor B has p_2 levels in the p_1xp_2 factorial and p_1 levels in the p_2xp_1 factorial.

Theorem 1.1 The rule for symmetry partitions a P^2 factorial into $k(k + 1)/2$ reduced symmetrical designs which are disjoint.

Proof: Each term in the expansion of $P^2 = (p_1 + p_2 + \ldots + p_k)^2$ represents a reduced symmetrical design. The number of terms in the expansion is $\binom{k}{1} + \binom{k}{2} = k(k + 1)/2$. Thomas (7) proves that each reduced factorial obtained from the above expansion is disjoint; that is, that there are no common points belonging to two or more reduced factorials. Since each reduced symmetrical design is either a reduced factorial or a combination of two reduced factorials, each is disjoint.

Denote the P levels of each factor by 1, 2, ..., P. Then the $p_1, p_2, \ldots, p_k$ levels selected from the original P levels, must be disjoint; that is, p_i can have no level in common with p_j for $i \neq j$, $i, j = 1, 2, \ldots, k$; and the selection must follow the procedure outlined below to obtain symmetrical designs. If we let φ^*_i represent the P x 1 vector of levels for the ith factor, and let $\varphi_{i1}, \varphi_{i2}, \ldots, \varphi_{ik}$ represent the $p_1 \times 1$, $p_2 \times 1$, ..., $p_k \times 1$ vectors of levels chosen for $p_1, p_2, \ldots, p_k$, respectively, then $\varphi^*_i = (\varphi'_{i1}, \varphi'_{i2}, \ldots \varphi'_{ik})$ gives a partitioning of the levels for the ith factor. We will assume $\varphi_{ir} = \varphi_{jr}$ for $i \neq j$ and $r = 1, 2, \ldots, k$. Hence, it is not necessary to use a subscript on φ to denote to which factor we are referring. It should also be noted that φ_1 does not necessarily represent the first p_1 levels of each factor, but any p_1 levels of each factor and similarly for $\varphi_2, \ldots, \varphi_k$.

In all subsequent discussions $p_i = 2$, $i = 1, \ldots, k-1$, and $p_k = 1$ if P is odd or $p_k = 2$ if P is even. Therefore to obtain symmetrical designs, the φ_i should be partitioned as follows: $\varphi_1 = (1,P)$, $\varphi_2 = (2,P-1)$, $\varphi_3 = (3,P-2)$, ..., $\varphi_k = (k,P-k+1) = (P/2, (P+2)/2)$ if P is even and $\varphi_k = (k) = ((P-1)/2)$ if P is odd. Thus P^2 could be expressed as

$$\left(\sum_{i=1}^{(P-1)/2} 2_i + 1\right)^2 \text{ for odd P and } \left(\sum_{i=1}^{P/2} 2_i\right)^2 \text{ for even P.}$$

<u>Example 2.2</u>: Consider a P^n factorial where P = 5, n = 2, $p_1 = 2$, $p_2 = 2$, and $p_3 = 1$. Then $(p_1 + p_2 + p_3)^2 = (2_1 + 2_2 + 1)^2 = 2_1^2 + 2_2^2 + 1^2 + 2(2_1 x 2_2^2) + 2\,(2_1 x 1) + 2\,(2_2 x 1)$. The 2's have been subscripted to relate them to the respective p_i. If we partition $\varphi'_0 = (1,5)$, $\varphi'_1 = (2,4)$, and $\varphi'_2 = (3)$, the six reduced symmetrical designs and their corresponding design points in terms of the original 5^2 treatment combinations are given in Table I.

TABLE I

REDUCED SYMMETRICAL DESIGNS OBTAINED FROM EXPANSION OF $(2_1 + 2_2 + 1)^2$

$2_1 x 2_1$	$2_2 x 2_2$	1x1	$2(2_1 x 2_2)$	$2(2_1 x 1)$	$2(2_2 x 1)$
(1,1) (1,5) (5,1) (5,5)	(2,2) (2,4) (4,2) (4,4)	(3,3)	(1,2) (2,1) (1,4) (4,1) (5,2) (2,5) (5,4) (4,5)	(1,3) (5,3) (3,1) (3,5)	(2,3) (4,3) (3,2) (3,4)

2.3 Optimality Criteria for Designs

If the i,j-th element of $(X'X)^{-1}$ is denoted by C_{ij}, then the covariance $(\hat{\beta}_i, \hat{\beta}_j)$ is $C_{ij}\ \sigma^2$. One of the criteria used to judge which of the possible symmetrical designs, F, with a given number of points N of a given P^n is optimal is that design which has the

$$\min_{f \epsilon F} \max_{\hat{\beta}_i} \{\text{var } \hat{\beta}_i\}_f .$$

A design which satisfies this is said to be minimax and to choose the minimax design, we first find the $\max_{\hat{\beta}_i}$ var $\hat{\beta}_i$ for each possible symmetrical design $f \epsilon F$ and then minimize this value over these designs F. The minimax design is the one which has the smallest maximum expected variance of the $\hat{\beta}_i$ and could be considered a conservative choice. It considers only the variances of the $\hat{\beta}_i$ and disregards the covariances of $(\hat{\beta}_i, \hat{\beta}_j)$.

A second optimality criterion of designs is called the minimum generalized variance. The minimum generalized variance design is obtained by finding

$$\min_{f \epsilon F} \left| (X'X)_f^{-1} \right| ,$$

where F denotes all possible designs for a specified number of points, N, and a specified number of levels, P. This criterion gives an "overall" measure of optimality in the sense that it is minimizing a function containing both the variances and covariances of the coefficients.

A third optimality criterion is called minimax characteristic root. The minimax characteristic root design is determined by finding

$$\min_{f \in F} \max_{r} \left[r \,\middle|\, \left| (X'X)_f^{-1} - rI \right| = 0 \right]$$

where r denotes a characteristic root of $(X'X)^{-1}$ and F denotes the same as above. This design is obtained by finding the minimum of maximum variances of uncorrelated linear functions of the $\hat{\beta}_i$'s over all designs $f \in F$.

A fourth criterion used to compare the goodness of designs is the minimum average variance $\hat{y}(u)$. This design has the minimum expected variance of $\hat{y}(u)$ over the whole region of experimentation. The formula for the average variance $\hat{y}(u)$ was determined for the square region, $-1 \leq x_i \leq 1$, $i = 1, 2$, and for the circular region, $0 \leq x_1^2 + x_2^2 \leq 1$. These formulae will be developed in Chapter III.

CHAPTER III

P^2 - WITH QUADRATIC MODEL

In this chapter we shall investigate the method of obtaining symmetrical designs from P^2 factorials where the design points will be chosen according to the rule for symmetry defined in Chapter II and will be used to estimate the coefficients, β_i, of the quadratic model

$$y(x_1, x_2) = \beta_0 x_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1^2 + \beta_4 x_1 x_2 + \beta_5 x_2^2 + \epsilon$$

where $-1 \leq x_i \leq 1$, $i = 1, 2$, $x_0 = 1$ and $\epsilon \sim$ NID $(0, \sigma^2)$. Designs which have an equal number of points, N, will be compared using the criteria of Chapter I to determine their "goodness" in estimating the quadratic model.

These designs can best be used in experiments which are of an investigative nature such as optimum seeking experiments or experiments used to determine the shape of a response surface in the region of a maximum response.

We shall now consider what designs are available and how they are obtained.

Referring to the rule for symmetry and to the expansion of $P^2 = (p_1 + p_2 + \ldots + p_k)^2$ given in Chapter I, it should be noted that all reduced symmetrical designs contain either four or eight-points with the exception of the one (center) point which occurs when P is odd. As P increases, the number of four and eight-point reduced symmetrical designs which are available increases; however the number of them depends on whether P is even or odd.

3.1 Case When P is Even

Theorem 3.1 The number of four-point factorials is P/2 and the number of eight-point factorials is P(P - 2)/8.

Proof: There are a total of $P^2 = (\sum_{i=1}^{p/2} 2_i)^2$ points available. From this expansion it is obvious that $2_1^2, 2_2^2, \ldots, 2_{p/2}^2$ are the four-point reduced symmetrical designs. Thus there are $\binom{P/2}{1} = P/2$ of these. The remaining terms indicate the eight-point reduced symmetrical designs and the number of these is $\binom{P/2}{2} = P(P - 2)/8$. Thus $4(P/2) + 8(P(P - 2)/8) = P^2$.

Example 3.1: Consider a P^2 factorial where P = 6. The $6^2 = 36$ points can be partitioned into 6/2 = 3 reduced symmetrical four-point designs and 6(6 - 2)/8 = 3 reduced symmetrical eight-point designs. Table II depicts these designs which have been denoted by 4_1, 4_2, 4_3, 8_1, 8_2, 8_3. Therefore the symmetrical designs of a 6^2 factorial are found by taking all combinations of the designs above. For example the four-point symmetrical designs are the 4_1, 4_2, 4_3; the eight-point symmetrical designs are 8_1, 8_2, 8_3, $4_1 + 4_2$, $4_1 + 4_3$ and $4_2 + 4_3$; and the twelve-point symmetrical designs are $8_1 + 4_1$, $8_1 + 4_2$, $8_1 + 4_3$, $8_2 + 4_1$, $8_2 + 4_2$, $8_2 + 4_3$, $8_3 + 4_1$, $8_3 + 4_2$ and $8_3 + 4_3$.

TABLE II

REPRESENTATION OF THE REDUCED SYMMETRICAL DESIGNS OBTAINABLE FROM A 6^2 FACTORIAL.*

LEVELS OF FACTOR B

LEVELS OF FACTOR A	1	2	3	4	5	6
1	4_1	8_1	8_2	8_2	8_1	4_1
2	8_1	4_2	8_3	8_3	4_2	8_1
3	8_2	8_3	4_3	4_3	8_3	8_2
4	8_2	8_3	4_3	4_3	8_3	8_2
5	8_1	4_2	8_3	8_3	4_2	8_1
6	4_1	8_1	8_2	8_2	8_1	4_1

*Different symbols indicate the reduced designs.

Using the different combinations of the reduced designs, the different N available for a 6^2 factorial are 4, 8, 12, 16, 20, 24, 28, 32 and 36 point symmetrical designs.

For each N there are several possible plans available, the number of plans depending upon N and P^2. There are $\binom{P^2}{N}$ possible ways to choose N points; but, when the condition of symmetry is applied, the number of ways to choose N points when P is even reduces to

$$f(N,\ P^2) = \sum_{(k_1,k_2)\epsilon K} \binom{P/2}{k_1}\binom{P(P-2)/8}{k_2} \qquad (1)$$

where $K = \{(k_1,k_2) \mid k_1, k_2$ are non-negative integral solutions to the equation $4k_1 + 8k_2 = N$ and $k_1 \leq P/2$ and $k_2 \leq P(P-2)/8\}$.

Example 3.2: Suppose we want the number of possible 16-point symmetrical plans available for a 6^2 factorial. Using (1) above, we find

$$f(16,\ 6^2) = \sum_{(k_1,\ k_2)\epsilon K} \binom{3}{k_1}\binom{3}{k_2} = \binom{3}{2}\binom{3}{1} + \binom{3}{0}\binom{3}{2} = 12.$$

where $K = \{(k_1, k_2) \mid k_1, k_2$ are non-negative integral solutions to $4k_1 + 8k_2 = 16$ and $k_1 \leq 3$ and $k_2 \leq 3\}$. Thus there are 12 different 16-point symmetrical plans for a 6^2 factorial. They are

$8_1 + 4_1 + 4_2$	$8_2 + 4_1 + 4_2$	$8_3 + 4_1 + 4_2$	$8_1 + 8_2$
$8_1 + 4_1 + 4_3$	$8_2 + 4_1 + 4_3$	$8_3 + 4_1 + 4_3$	$8_1 + 8_3$
$8_1 + 4_2 + 4_3$	$8_2 + 4_2 + 4_3$	$8_3 + 4_2 + 4_3$	$8_2 + 8_3$

3.2 Case When P is Odd

All reduced symmetrical designs are disjoint and are composed of either one, four or eight points depending upon the size of P.

Theorem 3.2 The number of one-point reduced designs is one; the number of four-point reduced designs in P - 1; and number of eight-point reduced designs is (P - 1)(P - 3)/8.

Proof: There are $P^2 = (\sum_{i=1}^{(P-1)/2} 2_i + 1)^2$ points available. From the expansion of P^2 it is obvious that 1^2 is the one-point design and $2_1^2, 2_2^2, \ldots, 2^2_{(P-1)/2}, 2(2_1 x1), 2(2_2 x1), \ldots, 2(2_{(P-1)/2} x1)$ are the $2\binom{(P-1)/2}{1} = P - 1$ four-point designs. The remaining terms indicate the eight-point designs and there are $\binom{(P-1)/2}{2} = (P-1)(P-3)/8$ of these. Thus $1 + 4\,(P-1) + 8\,((P-1)\,(P-3)/8) = P^2$.

Example 3.3: Consider a P^2 factorial where $P = 5$. The $5^2 = 25$ points may be partitioned into $5 - 1 = 4$ disjoint four-point designs and $(5 - 1)(5 - 3)/8 = 1$ disjoint eight-point design. Table III depicts these reduced designs which have been denoted by 1, 4_1, 4_2, 4_3, 4_4, 8. The different symmetrical designs available are found by taking all combinations of the reduced designs. Therefore the different N which may be obtained are 1, 4, 5, 8, 9, 12, 13, 16, 17, 20, 21, 24 and 25 point symmetrical designs. For example, the four-point symmetrical designs are 4_1, 4_2, 4_3 and 4_4; the nine-point symmetrical designs are $4_1 + 4_2 + 1$, $4_1 + 4_3 + 1$, $4_1 + 4_4 + 1$, $4_2 + 4_3 + 1$, $4_2 + 4_4 + 1$, $4_3 + 4_4 + 1$ and $8 + 1$.

TABLE III

REPRESENTATION OF THE REDUCED SYMMETRICAL DESIGNS OBTAINABLE FROM A 5^2 FACTORIAL.*

LEVELS OF FACTOR B

LEVELS OF FACTOR A	1	2	3	4	5
1	4_1	8	4_3	8	4_1
2	8	4_2	4_4	4_2	8
3	4_3	4_4	1	4_4	4_3
4	8	4_2	4_4	4_2	8
5	4_1	8	4_3	8	4_1

*Different symbols represent the disjoint groups.

The number of possible symmetrical plans for a particular N when P is odd is

$$f(N,P^2) = \sum_{(k_1,k_2)\in K} \binom{P-1}{k_1}\binom{(P-1)(P-3)/8}{k_2} \qquad (2)$$

where $K = \{(k_1,k_2) | k_1,k_2$ are non-negative integral solutions to the equation $4k_1 + 8k_2 = N$ when N is even and to the equation $4k_1 + 8k_2 = N - 1$ when N is odd and $k_1 \leq P - 1$ and $k_2 \leq (P - 1)(P - 3)/8\}$.

Example 3.4: Suppose we want the number of 13-point symmetrical plans available for a 5^2 factorial. Using (2) above, we find

$$f(13,5^2) = \sum_{(k_1,k_2)\varepsilon K} \binom{4}{k_1}\binom{1}{k_2} = \binom{4}{3}\binom{1}{0} + \binom{4}{1}\binom{1}{1} = 8.$$

where $K = \{(k_1,k_2) | k_1,k_2$ are non-negative integral solutions to $4k_1 + 8k_2 = 12$ and $k_1 \leq 4$ and $k_2 \leq 1\}$. Thus there are 8 different 13-point symmetrical plans for a 5^2 factorial. They are

$$\begin{array}{llll} 8 + 4_1 + 1 & 8 + 4_3 + 1 & 4_1 + 4_2 + 4_3 + 1 & 4_1 + 4_3 + 4_4 + 1 \\ 8 + 4_2 + 1 & 8 + 4_4 + 1 & 4_1 + 4_2 + 4_4 + 1 & 4_2 + 4_3 + 4_4 + 1. \end{array}$$

We now have a method for determining the number of different N-point designs which may be used and the number of plans available for each N. We shall now proceed to determine which of these plans is optimal for specified N and P^2.

CHAPTER IV

OPTIMAL DESIGNS FOR P^2 WITH QUADRATIC MODEL

In this chapter we shall demonstrate the designs which are optimal for some specified N and P^2, the procedure by which these optimal designs were chosen, the plans for these optimal designs, and the optimal designs for specified N as we let P vary to infinity.

We assumed earlier that all design points would be coded into the region $-1 \leq x_i \leq 1$. Using this assumption we can determine <u>a priori</u> the values for the X matrix when a symmetrical plan is chosen.

<u>Example 4.1</u>: Consider a P^2 factorial when $P = 5$. Thus the i-th factor has five levels and they are $X_{i1} = -1.0$, $X_{i2} = -0.5$, $X_{i3} = 0$, $X_{i4} = 0.5$, and $X_{i5} = 1.0$.

<u>4.1 Procedures Used to Determine the Optimal Designs</u>

Now let us consider the procedure by which these optimal designs were chosen. Using the quadratic model we can determine the values for (X'X) and $(X'X)^{-1}$ in terms of the coded design points, $X^* = (X_{1i}, X_{2j})$. Thus

$$(X'X)_f = \begin{bmatrix} \Sigma x_{01}^2 & 0 & 0 & \Sigma x_{1i}^2 & 0 & \Sigma x_{2i}^2 \\ 0 & \Sigma x_{1i}^2 & 0 & 0 & 0 & 0 \\ 0 & 0 & \Sigma x_{2i}^2 & 0 & 0 & 0 \\ \Sigma x_{1i}^2 & 0 & 0 & \Sigma x_{1i}^4 & 0 & \Sigma x_{1i}^2 x_{2i}^2 \\ 0 & 0 & 0 & 0 & \Sigma x_{1i}^2 x_{2i}^2 & 0 \\ \Sigma x_{2i}^2 & 0 & 0 & \Sigma x_{1i}^2 x_{2i}^2 & 0 & \Sigma x_{2i}^4 \end{bmatrix}$$

Let $a = \Sigma x_{0i}^2 = N$, $b = \Sigma x_{1i}^2 = \Sigma x_{2i}^2$, $c = \Sigma x_{1i}^4 = \Sigma x_{2i}^4$, $d = \Sigma x_{1i}^2 x_{2i}^2$.

Then

$$(X'X)_f^{-1} = \begin{bmatrix} C_{11} & 0 & 0 & C_{14} & 0 & C_{16} \\ 0 & C_{22} & 0 & 0 & 0 & 0 \\ 0 & 0 & C_{33} & 0 & 0 & 0 \\ C_{41} & 0 & 0 & C_{44} & 0 & C_{46} \\ 0 & 0 & 0 & 0 & C_{55} & 0 \\ C_{61} & 0 & 0 & C_{64} & 0 & C_{66} \end{bmatrix}$$

where $C_{11} = (c + d)/[N(c + d) - 2b^2]$,

$C_{22} = C_{33} = 1/b$,

$C_{44} = C_{66} = (Nc - b^2)/(c - d)[N(c + d) - 2b^2]$,

$C_{55} = 1/d$,

$C_{14} = C_{16} = C_{41} = C_{61} = -b/[N(c + d) - 2b^2]$,

$C_{46} = C_{64} = (b^2 - Nd)/(c - d)[N(c + d) - 2b^2]$.

The procedure for determining the <u>minimax design</u> may now be expressed as

$$\min_{f \epsilon F} \max_{\hat{\beta}} [\mathrm{var}\ \hat{\beta}]_f = \min_{f \epsilon F} \max_{C_{ii}} [C_{ii},\ i = 1, \ldots, 6]_f$$

where F denotes the set of all symmetrical designs for N points.

The <u>minimum generalized variance design</u> is defined as

$$\min_{f \epsilon F} \left| (X'X)_f^{-1} \right| = \max_{f \epsilon F} \left| (X'X)_f \right|$$

where F is defined above. This can be expressed as

$$\max_{f \epsilon F} \{b^2 d(c - d)[N(c + d) - 2b^2]\}_f = \min_{f \epsilon F} \{1/(b^2 d(c - d)[N(c + d) - 2b^2])\}_f$$

The minimax characteristic root design is defined as

$$\min_{f \in F} \max_{r} \{r \,|\, |(X'X)_f^{-1} - rI| = 0\}$$

where r denotes a characteristic root of $(X'X)_f^{-1}$ and F is defined above. Solving the equation

$$\begin{aligned}
|(X'X)_f^{-1} - rI| &= (C_{22} - r)^2 (C_{55} - r)[(C_{11} - r)(C_{44} - r)^2 + 2C_{14}^2 C_{46} \\
&\quad - 2C_{14}^2 (C_{44} - r) - C_{46}^2 (C_{11} - r)] \\
&= (C_{22} - r)^2 (C_{55} - r)(C_{44} - C_{46} - r) \\
&\quad [(C_{11} - r)(C_{44} + C_{46} - r) - 2C_{14}^2] = 0.
\end{aligned}$$

we find there are six characteristic roots of $(X'X)_f^{-1}$ which may be denoted by

$$\begin{aligned}
r_1 &= r_2 = C_{22}, \\
r_3 &= C_{55}, \\
r_4 &= C_{44} - C_{46}, \\
r_5 &= \{C_{11} + C_{44} + C_{46} + [(C_{11} - C_{44} - C_{46})^2 + 8C_{14}^2]^{1/2}\}/2, \\
r_6 &= \{C_{11} + C_{44} + C_{46} - [(C_{11} - C_{44} - C_{46})^2 + 8C_{14}^2]^{1/2}\}/2.
\end{aligned}$$

4.2 Optimal Designs for Specified N and P^2

All possible symmetrical designs with N = 8, 9, 12, 13 and P = 3, ..., 50 were determined with the aid of a high speed computer and the designs which were optimal with respect to estimating the quadratic, two-dimensional model $y(x_1, x_2)$ were chosen according to the procedures defined above. A total of 552 optimal designs was obtained for which some are exhibited here. The optimal designs for which N = 8, 9, 13, P = 5, 7, 9 and N = 12, P = 4, ..., 9, were chosen to be exhibited in Tables IV, V and VI. These are all the possible values of N available for N < 16.

Now we want to determine, for a fixed N, the design which is optimal when there are no restrictions on the number of levels, P, for each factor. As P increases to infinity, the values of the points for each optimal design approach a limiting value. To clarify how these optimal limiting designs are determined, let us consider the minimax design for 9 points. The minimax design was obtained by comparing all possible 9-point symmetrical designs for each P = 3, 5, ..., 49. A trend as P increased which gave an indication of the limiting positions which the points were approaching was established. Some points remained fixed as P increased. Therefore using the form indicated by the trend and the points which were changing, M, as a variable, we were able to solve for the value of the points which would produce the optimal design as P approached infinity.

The symmetrical design satisfying each optimality criterion for each N was determined for each P = 3, ..., 50, involving the analysis of over five hundred thousand different plans. The trends of these optimal designs were established which resulted in the following theorems.

4.3 Minimax Designs as $P \to \infty$

Theorem 4.1 If N = 8, P is odd and if the limiting points are (1, 1), (1, -1), (-1, 1), (-1, -1), (M, 0), (0, M), (-M, 0), (0, -M), then the minimax design occurs at M = 0.87560077 as P approaches infinity.

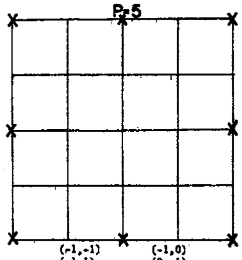
Proof: The diagonal elements of $(X'X)^{-1} = (C_{ij})$ are the values compared to determine the minimax design. These values, as a function of M, are

TABLE IV

MINIMAX DESIGNS FOR SPECIFIED N AND P^2

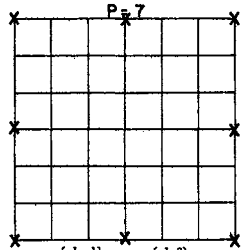
N = 8

P = 5



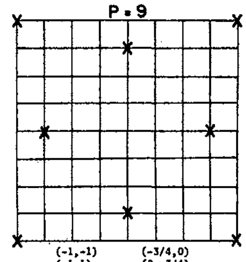
(-1,-1) (-1,0)
(-1,1) (0,-1)
(1,-1) (0,1)
(1,1) (1,0)

P = 7



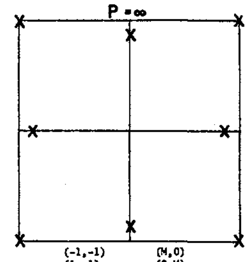
(-1,-1) (-1,0)
(-1,1) (0,-1)
(1,-1) (0,1)
(1,1) (1,0)

P = 9



(-1,-1) (-3/4,0)
(-1,1) (0,-3/4)
(1,-1) (3/4,0)
(1,1) (0,3/4)

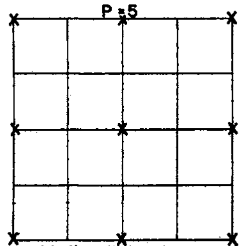
P = ∞



(-1,-1) (M,0)
(1,-1) (0,M)
(-1,1) (-M,0)
(1,1) (0,-M)
M = 0.875600765

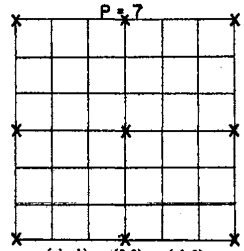
N = 9

P = 5



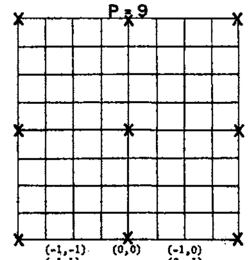
(-1,-1) (0,0) (-1,0)
(-1,1) (0,-1)
(1,-1) (1,0)
(1,1) (0,1)

P = 7



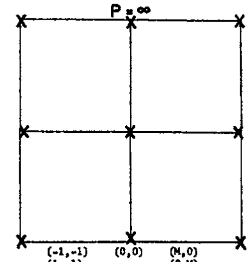
(-1,-1) (0,0) (-1,0)
(-1,1) (0,-1)
(1,-1) (1,0)
(1,1) (0,1)

P = 9



(-1,-1) (0,0) (-1,0)
(-1,1) (0,-1)
(1,-1) (1,0)
(1,1) (0,1)

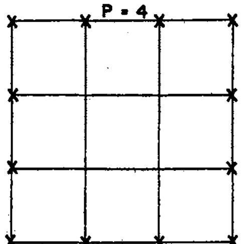
P = ∞



(-1,-1) (0,0) (M,0)
(1,-1) (0,M)
(1,1) (-M,0)
(-1,1) (0,-M)
M = 0.97062299

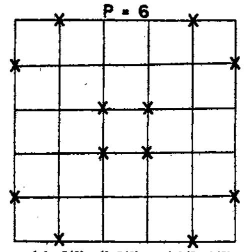
N = 12

P = 4



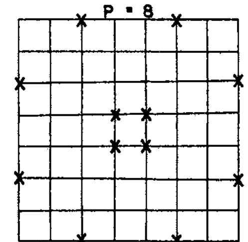
(-1,-1/3) (1,1/3) (-1,-1)
(-1,1/3) (-1/3,-1) (-1,1)
(1/3,-1) (-1/3,1) (1,-1)
(1/3,1) (1,-1/3) (1,1)

P = 6



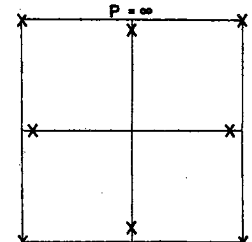
(-1,-3/5) (1,3/5) (-1/5,-1/5)
(-1,3/5) (3/5,1) (-1/5,1/5)
(3/5,-1 (-3/5,1) (1/5,-1/5)
(-3/5,-1) (1,-3/5) (1/5,1/5)

P = 8



(-1,-3/7) (-3/7,1) (-1/7,-1/7)
(-3/7,-1) (1,-3/7) (-1/7,1/7)
(3/7,-1) (3/7,1) (1/7,-1/7)
(-1,3/7) (1,3/7) (1/7,1/7)

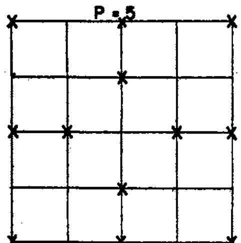
P = ∞



(-1,-1) (M,0) (-M,0)
(1,-1) (M,0) (-M,0)
(-1,1) (0,M) (0,-M)
(1,1) (0,M) (0,-M)
M = 0.89309748

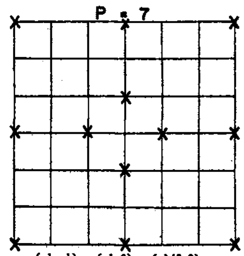
N = 12

P = 5



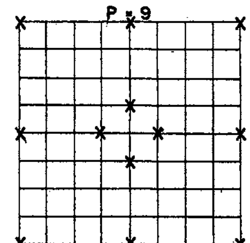
(-1,-1) (-1,0) (-1/2,0)
(-1,1) (0,-1) (0,-1/2)
(1,-1) (1,0) (0,1/2)
(1,1) (0,1) (1/2,0)

P = 7



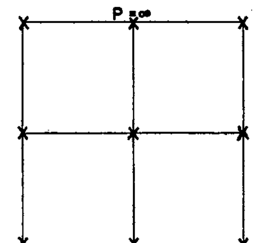
(-1,-1) (-1,0) (-1/3,0)
(-1,1) (0,-1) (0,-1/3)
(1,-1) (1,0) (0,1/3)
(1,1) (0,1) (1/3,0)

P = 9



(-1,-1) (-1,0) (-1/4,0)
(-1,1) (0,-1) (0,-1/4)
(1,-1) (0,1) (0,1/4)
(1,1) (1,0) (1/4,0)

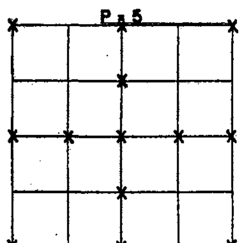
P = ∞



(-1,-1) (-1,0) (0,0)
(1,-1) (0,-1) (0,0)
(-1,1) (0,1) (0,0)
(1,1) (1,0) (0,0)

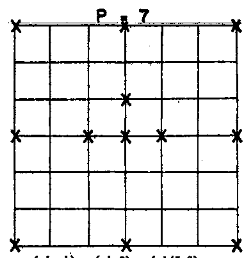
N = 13

P = 5



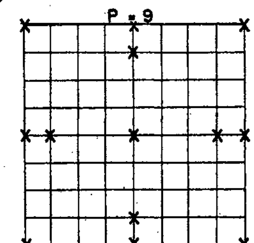
(-1,-1) (-1,0) (-1/2,0)
(-1,1) (0,-1) (0,-1/2)
(1,-1) (0,1) (0,1/2)
(1,1) (1,0) (1/2,0)
(0,0)

P = 7



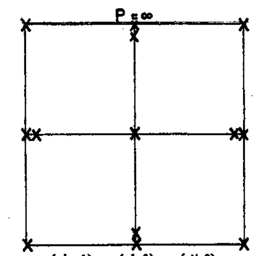
(-1,-1) (-1,0) (-1/3,0)
(-1,1) (0,-1) (0,-1/3)
(1,-1) (0,1) (0,1/3)
(1,1) (1,0) (1/3,0)
(0,0)

P = 9



(-1,-1) (-1,0) (-3/4,0)
(-1,1) (0,-1) (0,-3/4)
(1,-1) (1,0) (3/4,0)
(1,1) (0,1) (0,3/4)
(0,0)

P = ∞



(-1,-1) (-1,0) (-M,0)
(-1,1) (0,-1) (0,-M)
(1,-1) (1,0) (M,0)
(1,1) (0,1) (0,M)
(0,0)
M = 0.89255196

TABLE V

MINIMUM GENERALIZED VARIANCE DESIGNS FOR SPECIFIED N AND P^2

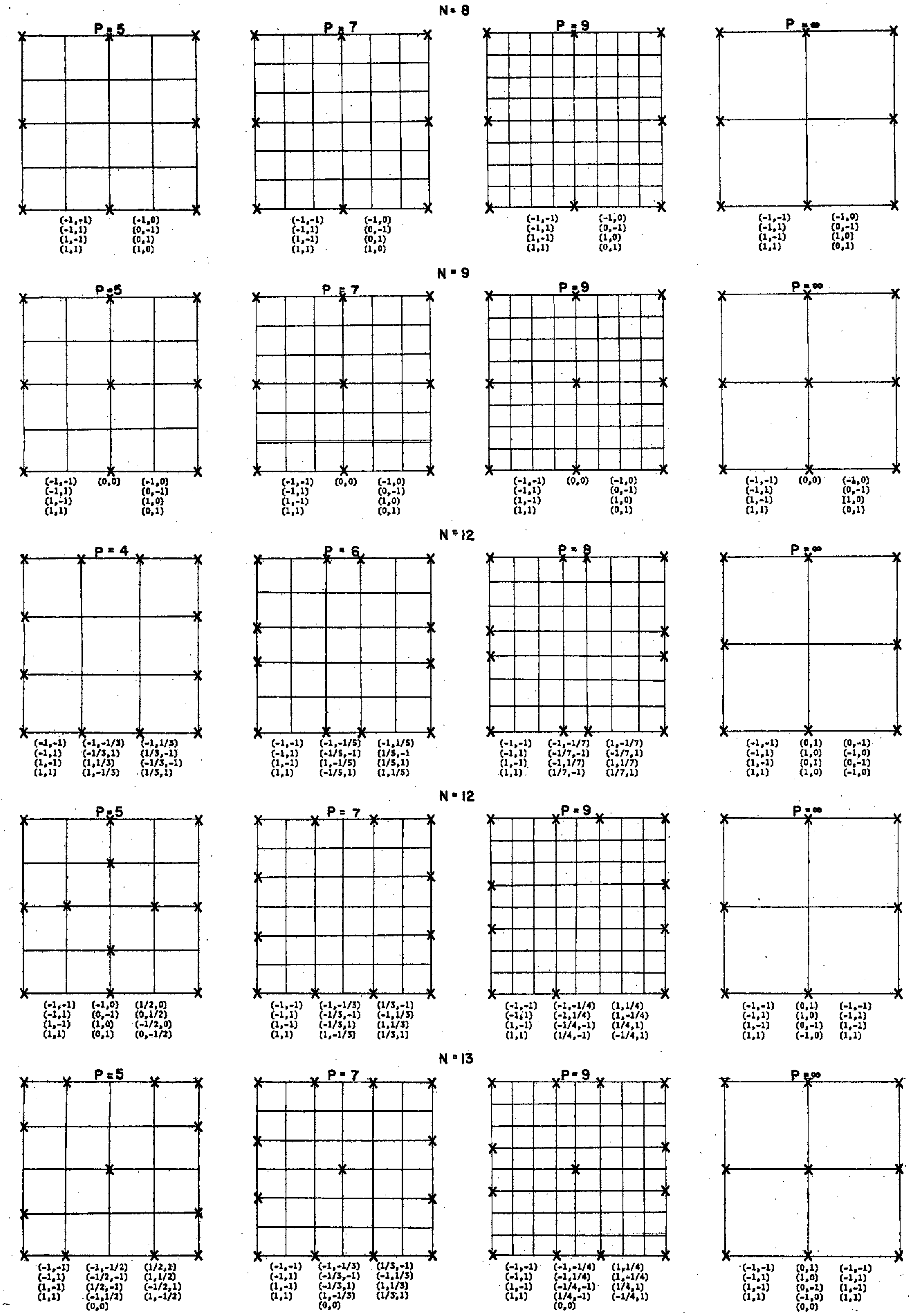
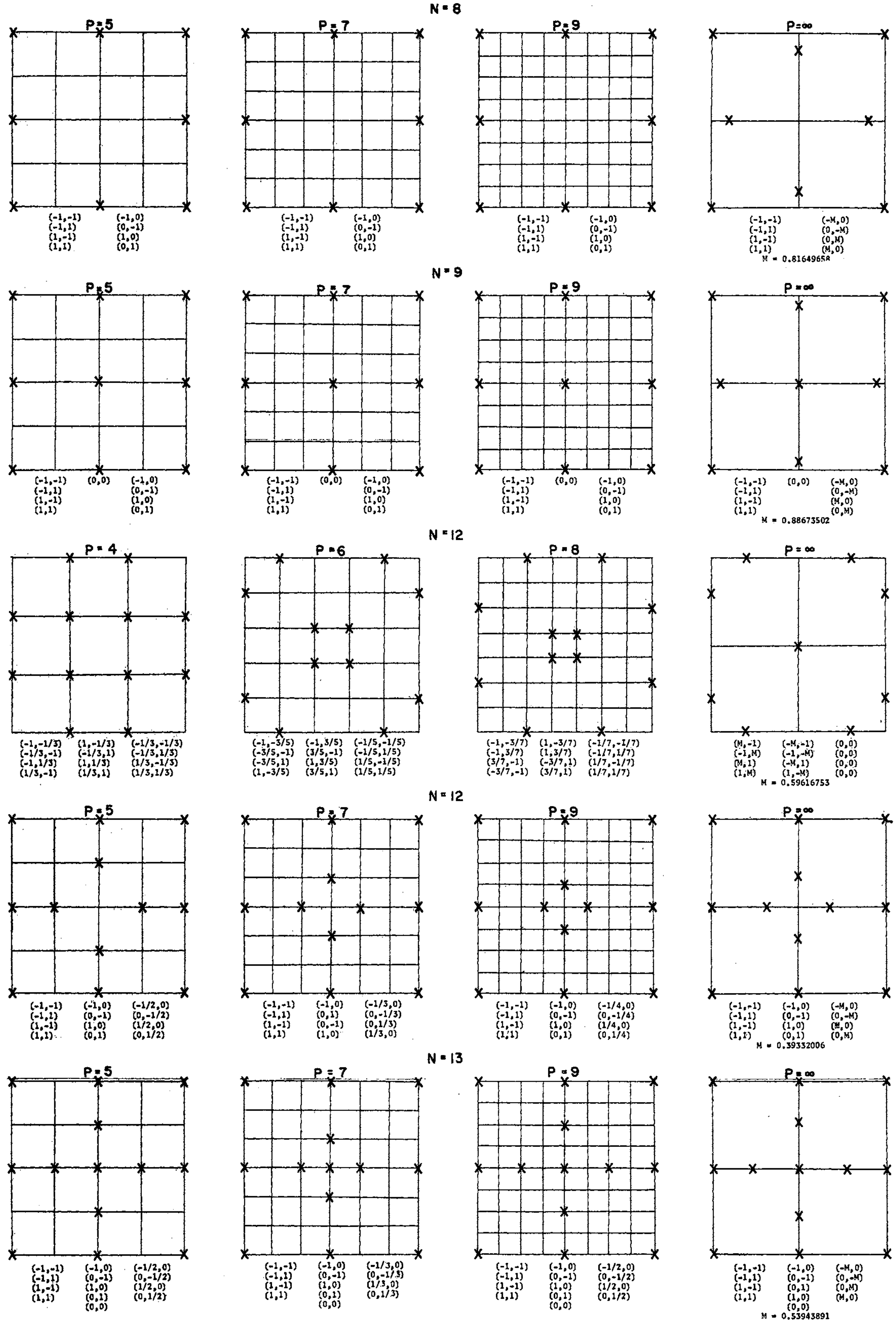


TABLE VI

MINIMAX CHARACTERISTIC ROOT DESIGNS FOR SPECIFIED N AND P^2



$$C_{11} = (4 + M^4)/4(2 - M^2)^2,$$
$$C_{22} = C_{33} = 1/(4 + 2M^2),$$
$$C_{44} = C_{66} = (4 - 4M^2 + 3M^4)/4M^4(2 - M^2)^2,$$
$$C_{55} = 1/4.$$

It is obvious that C_{11} and C_{44} are greater than or equal to C_{22} and C_{55} in [0, 1]. By examining the equations for C_{11} and C_{44} we see that the minimax value occurs at the intersection of C_{11} and C_{44}. Therefore by setting $C_{11} = C_{44}$, we obtain an equation of the form $M^8 + M^4 + 4M^2 - 4 = 0$ which has a solution in [0,1] which is $M = (0.7666767)^{1/2} = 0.87560077$. If P = 1001, then M would be 63 divisions from the edge of the region.

<u>Theorem 4.2</u> If N = 9, P is odd and if the limiting points are (1, 1), (-1, 1), (1, -1), (-1, -1), (0, 0), (M, 0), (0, M), (-M, 0), (0, -M), then the minimax design occurs at M = 0.97062299 as $P \rightarrow \infty$.

<u>Proof</u>: The same properties for C_{11} and C_{44} exist here as in Theorems 4.1. Therefore by setting $C_{11} = C_{44}$ and solving for the point of intersection, we obtain an equation of the form $2M^8 + M^4 + 8M^2 - 10 = 0$ which has a solution in [0,1] which is $M = (0.942109)^{1/2} = 0.97962299$.

<u>Theorem 4.3</u> If N = 12, P is odd and if the limiting points are (1, 1), (1, -1), (-1, 1), (-1, -1), (1, 0), (-1, 0), (0, 1), (0, -1), (M, 0), (0, M), (-M, 0), (0, -M), then the minimax design occurs at M = 0.0 as $P \rightarrow \infty$.

<u>Proof</u>: The properties of C_{11} and C_{44} are the same as in Theorem 4.1 except for the forms of the equations. Upon obtaining dC_{11}/dM and dC_{44}/dM, we find that C_{11} and C_{44} are monotonic increasing functions of M from which we conclude that M = 0.0 is the value which is necessary to produce the minimax design for 12 points.

Theorem 4.4 If $N = 12$, P is even and if the limiting points are (1, 1), (1, -1), (-1, 1), (-1, -1), (M, 0), (0, M), (M, 0), (0, M), (-M, 0), (0, -M), (-M, 0), (0, -M), then the minimax design occurs at $M = 0.89309748$ as $P \to \infty$.

Proof: The same properties for C_{11} and C_{44} exist here as in Theorem 4.1. Therefore by setting $C_{11} = C_{44}$ and solving for the point of intersection, we obtain an equation of the form $M^8 + 2M^2 - 2 = 0$ which has a solution in $[0,1]$ at $M = 0.89309748$.

Theorem 4.5 If $N = 13$, P is odd and if the limiting points are (1, 1), (1, -1), (-1, 1), (-1, -1), (1, 0), (0, 1), (-1, 0), (0, -1), (0, 0), (0, M), (M, 0), (0, -M), (-M, 0), then the minimax design occurs at $M = 0.89255196$ as $P \to \infty$.

Proof: The same properties for C_{11} and C_{44} exist here as in Theorem 4.1. By solving for the intersection we obtain an equation of the form $2M^8 + M^4 + 12M^2 + 11 = 0$ which has a solution in $[0,1]$ at $M = 0.89255196$.

4.4 Minimum Generalized Variance Designs as $P \to \infty$

Theorem 4.6 If $N = 8$, P is odd and if the limiting points are (1, 1), (1, -1), (-1, 1), (-1, -1), (M, 0), (0, M), (-M, 0), (0, -M), then the minimum generalized variance design occurs at $M = 1$ as $P \to \infty$.

Proof: If the points (1, 1), (1, -1), (-1, 1), (-1, -1), (M, 0), (0, M), (-M, 0), (0, -M) are chosen, then $|(X'X)^{-1}| = [64M^4(2 + M^2)^2(2 - M^2)^2]^{-1}$. Upon taking the derivative of the determinant with respect to M, we find that the $|(X'X)^{-1}|$ is a monotonic decreasing function of M and therefore has a minimum in $[0,1]$ at $M = 1$.

<u>Theorem 4.7</u> If $N = 9$, P is odd and the limiting points are $(1, 1)$, $(1, -1)$, $(-1, 1)$, $(-1, -1)$, $(M, 0)$, $(0, M)$, $(-M, 0)$, $(0, -M)$, $(0, 0)$, then the minimum generalized variance design occurs at $M = 1$ as $P \rightarrow \infty$.

<u>Proof</u>: The proof is the same as the proof of Theorem 4.6 with the exception that $|(X'X)^{-1}| = [64M^4(2 + M^4)^2(20 - 16M^2 + 5M^4)]^{-1}$.

<u>Theorem 4.8</u> If $N = 12$, P is even and if the limiting points are $(1, 1)$, $(1, -1)$, $(-1, 1)$, $(-1, -1)$, $(-1, M)$, $(M, -1)$, $(1, M)$, $(M, 1)$, $(-1, -M)$, $(-M, -1)$, $(1, -M)$, $(-M, 1)$, then the minimum generalized variance design occurs at $M = 0$ as $P \rightarrow \infty$.

<u>Proof</u>: The $|(X'X)^{-1}| = [16^3(2 + M^2)^2(1 + 2M^2)(1 - M^2)^4]^{-1}$ is a monotonic increasing function of M in $[0,1]$ and therefore attains a minimum at $M = 0$.

<u>Theorem 4.9</u> If $N = 12$, P is odd and if the limiting points are $(1, 1)$, $(1, -1)$, $(-1, 1)$, $(-1, -1)$, $(1, 0)$, $(0, 1)$, $(-1, 0)$, $(0, -1)$, (M, M), $(M, -M)$, $(-M, M)$, $(-M, -M)$, then the minimum generalized variance design occurs at $M = 1$ as $P \rightarrow \infty$.

<u>Proof</u>: The $|(X'X)^{-1}| = [512(3 + 2M^2)^2(1 + M^4)(3 - 6M^2 + 4M^4)]^{-1}$ is a decreasing function of M in $[0,1]$ and therefore attains a minimum at $M = 1$. The above points produce the minimum generalized variance design for $P = 31, 33, \ldots, \infty$. Due to the finiteness of the values of M, for $P = 5, 7, \ldots, 29$, the points which produce the optimum are $(1, 1)$, $(1, -1)$, $(-1, 1)$, $(-1, -1)$, $(1, M)$, $(M, 1)$, $(1, -M)$, $(-M, 1)$, $(-1, M)$, $(M, -1)$, $(-1, -M)$, $(-M, -1)$, where M is a value close to zero for each P. For these points $|(X'X)^{-1}| = [16^3(2 + M^2)^2(1 + 2M^2)(1 - M^2)^4]^{-1}$.

<u>Theorem 4.10</u> If $N = 13$, P is odd and if the limiting points are (1, 1), (1, -1), (-1, 1), (-1, -1), (1, 0), (0, 1), (-1, 0), (0, -1), (0, 0), (M, M), (M, -M), (-M, M), (-M, -M), then the minimum generalized variance design occurs at $M = 1$ as $P \to \infty$.

<u>Proof</u>: The $|(X'X)^{-1}| = [32(3 + 2M^2)^2(1 + M^4)(58 - 96M^2 + 72M^4)]^{-1}$ is a decreasing function of M in [0,1] and therefore the minimum occurs at $M = 1$ as $P \to \infty$.

4.5 Minimax Characteristic Root Designs as $P \to \infty$

<u>Theorem 4.11</u> If $N = 8$, P is odd and if the limiting points are (1, 1), (1, -1), (-1, 1), (-1, -1), (M, 0), (0, M), (-M, 0), (0, -M), then the minimax characteristic root design occurs at $M = 0.81649658$ as $P \to \infty$.

<u>Proof</u>: There are six characteristic roots of $(X'X)^{-1}$ which, in this case, have equations of the form

$$r_1 = r_2 = 1/(4 + 2M^2),$$
$$r_3 = 1/4,$$
$$r_4 = 1/2M^4,$$
$$r_5 = 1/[8 + M^4 + (32 + 32M^2 + 8M^4 + M^8)^{1/2}],$$
$$r_6 = 1/[8 + M^4 - (32 + 32M^2 + 8M^4 + M^8)^{1/2}].$$

Since we desire the minimax of the r_i, it is necessary to consider only r_4, a monotonic decreasing function of M, and r_6 a monotonic increasing function of M, because they are greater than the other r_i in [0,1]. We are looking for the minimum of the maximums which occurs at the intersection of r_4 with r_6 and the value of M at this intersection is $M = 0.81649658$ as $P \to \infty$.

<u>Theorem 4.12</u> If $N = 9$, P is odd and if the limiting points are (1, 1), (1, -1), (-1, 1), (-1, -1), (0, 0), (M, 0), (0, M), (-M, 0), (0, -M), then the minimax characteristic root design occurs at $M = 0.88673502$ as $P \to \infty$.

<u>Proof</u>: The proof is similar to that for Theorem 4.11 with the exception that r_5 and $r_6 = [17 + 2M^4 \pm (129 + 128M^2 + 28M^4 + 4M^8)^{1/2}]^{-1}$.

<u>Theorem 4.13</u> If $N = 12$, P is even and if the limiting points are (1, M), (M, 1), (1, -M), (-M, 1), (M, -1), (-1, M), (-1, -M), (-M, -1), (0, 0), (0, 0), (0, 0), (0, 0), then the minimax characteristic root design occurs at $M = 0.59616753$ as $P \to \infty$.

<u>Proof</u>: The proof is similar to that for Theorem 4.11 with the exception that $r_3 = 1/8M^2$ and r_5, $r_6 = \{2[4 + 2M^2 + M^4 \pm (12 + 8M^2 + 8M^4 + 4M^6 + M^8)^{1/2}]\}^{-1}$.

<u>Theorem 4.14</u> If $N = 12$, P is odd and if the limiting points are (1, 1), (1, -1), (-1, 1), (-1, -1), (1, 0), (0, 1), (-1, 0), (0, -1), (M, 0), (0, M), (-M, 0), (0, -M), then the minimax characteristic root design occurs at $M = 0.39332005$ as $P \to \infty$.

<u>Proof</u>: The proof is similar to that for Theorem 4.11 with the exception that r_5, $r_6 = [11 + M^4 \pm (73 + 48M^2 + 6M^4 + M^8)^{1/2}]^{-1}$.

<u>Theorem 4.15</u> If $N = 13$, P is odd and if the limiting points are (1, 1), (1, -1), (-1, 1), (-1, -1), (0, 0), (1, 0), (0, 1), (-1, 0), (0, -1), (M, 0), (0, M), (-M, 0), (0, -M), then the minimax characteristic root design occurs at $M = 0.53943890$ as $P \to \infty$.

Proof: The proof is similar to that for Theorem 4.11.

In each of the preceeding theorems we have solved for a value of $\bar{M}$. To relate the value of M to the partitions of the region $-1 \leq x_i \leq 1$ and to letting $P \to \infty$, we can use the relationship $(P + 1 - 2i)/(P - 1) = M$ where i is the number of partitions from the boundary of the region. The values for M are discrete for any value of $P < \infty$. As $P \to \infty$, M becomes continuous and enables us to determine the limiting values for each of the optimal designs.

It should be noted that for 12-point designs we obtain different limiting designs depending on whether P is odd or even as $P \to \infty$. This happens because there are different designs available for even and odd P. When comparing the 12-point limiting design for odd P with the 12-point limiting design for even P, we find that the 12-point limiting design for odd P satisfies the three optimality criteria we have been discussing.

Let us abbreviate minimax, minimum generalized variance and minimax characteristic root as MM, MGV and MCR, respectively, for the following discussion.

Some interesting results were observed for these optimality criteria. The four corner points occurred in every optimal design with exception of six 12-point designs where P was even. The remaining points varied according to the value of N and the optimality criteria used. For the limiting designs the following results were observed.

For N = 8 and N = 9, the MM and MCR designs were very similar, having four corner points and four points having the shape of a diamond with a radius approximately equal to one.

For N = 12 and an odd P, the MM design had four corner points, four points which had the shape of a diamond with a radius equal to one and four center points. The MGV design had two points at each of the four corners and four points which had the shape of a diamond with a radius equal to one. The MCR design had four corner points, four points which had the shape of a diamond with a radius equal to one and four points in a diamond shape with a radius approximately equal to 0.4.

For N = 13, the results were very similar to the results for N = 12 except that the center point was added.

All the MGV designs had the same points; however, some were replicated more than others depending upon N. The points were all on the edge of the region of experimentation with the exception of the center point when N was odd.

It should be noted that the rotatable central composite design (9-point design with P = 5) did not satisfy any of the optimality criteria.

CHAPTER V

AVERAGE VARIANCE OF THE ESTIMATED RESPONSE

In this chapter we will be concerned with determining the average variance of the estimated response $\hat{y}(u_1, u_2)$, using symmetrical designs, in the two-dimensional case, for any distribution of the total probability mass to the region of interest; namely, the square region

$$R = [(u_1, u_2) \mid -1 \leq u_i \leq 1; i = 1, 2],$$

and the circular region

$$R_c = [(u_1, u_2) \mid u_1^2 + u_2^2 \leq 1].$$

In either case, assume the quadratic model

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1^2 + \beta_4 x_1 x_2 + \beta_5 x_2^2 + \varepsilon.$$

Folks (1) determined the average variance of $\hat{y}(u_1, u_2)$ under the assumptions of a linear model and that every point in the region of interest was assigned equal probability mass with no restrictions as to where the points were to be placed. Gillett (3) determined the average variance of $\hat{y}(u_1, u_2)$ under the assumption of a linear model and of any distribution of the total probability mass to n different subregions of interest with no restriction as to where the points were to be placed.

Let us now determine the formulae for the average variance of $\hat{y}(u_1, u_2)$ in the regions R and R_c.

5.1 Average Variance of $\hat{y}(u_1, u_2)$ in R and R_c

Theorem 5.1 If the total probability mass M = 1 is assigned to the n subregions

$$R_i = [(u_1, u_2) \mid -a_i \leq u_j \leq a_i;\ j = 1, 2] - R_{i-1}$$

($i = 1, 2, \ldots, n$; $R_0 = \varphi$, $a_0 = 0$), of the region R, then the average variance of $\hat{y}(u_1, u_2)$ over R is given by

$$\begin{aligned}\text{ave var } \hat{y}(u_1, u_2) = \text{var } \hat{\beta}_0 + \sum_{i=1}^{n} M_i \{(1/3)[\text{var } \hat{\beta}_1 + \text{var } \hat{\beta}_2 \\ + 4 \text{ cov } (\hat{\beta}_0, \hat{\beta}_3)](a_i^2 + a_{i-1}^2) + [(1/5)(\text{var } \hat{\beta}_3 + \text{var } \hat{\beta}_5) \\ + (1/9)(\text{var } \hat{\beta}_4 + 2 \text{ cov } (\hat{\beta}_3, \hat{\beta}_5))][a_i^4 + a_i^2 a_{i-1}^2 + a_{i-1}^4]\},\end{aligned}$$

where M_i denotes the probability mass assigned to R_i and $\sum_{i=1}^{n} M_i = 1$.

Proof: Let

$$A_i = (2a_i)^2 - (2a_{i-1})^2$$

be the area of R_i ($i = 1, 2, \ldots, n$; $a_0 = 0$), then $f_i(u_1, u_2) = K_i$, where

$$\begin{aligned} K_i &= M_i/A_i \text{ if } (u_1, u_2) \in R_i \\ &= 0 \qquad \text{otherwise} \end{aligned}$$

defines the value of the density function f_i at each (u_1, u_2) in R. Thus

$$\begin{aligned}\text{ave var } \hat{y}(u_1, u_2) = \sum_{i=1}^{n} [\int_{-a_i}^{a_i}\int_{-a_i}^{a_i} \text{var } \hat{y}(u_1, u_2) f_i(u_1, u_2) du_1\, du_2 \\ - \int_{-a_{i-1}}^{a_{i-1}}\int_{-a_{i-1}}^{a_{i-1}} \text{var } \hat{y}(u_1, u_2) f_i(u_1, u_2) du_1\, du_2]\end{aligned}$$

$$\begin{aligned}= \sum_{i=1}^{n} K_i \{\int_{-a_i}^{a_i}\int_{-a_i}^{a_i} [\text{var } \hat{\beta}_0 + u_1^2 \text{ var } \hat{\beta}_1 + u_2^2 \text{ var } \hat{\beta}_2 + u_1^4 \text{ var } \hat{\beta}_3 + u_1^2 u_2^2 \text{ var } \hat{\beta}_4 \\ + u_2^4 \text{ var } \hat{\beta}_5 + 2u_1^2 \text{ cov } (\hat{\beta}_0, \hat{\beta}_3) + 2u_2^2 \text{ cov } (\hat{\beta}_0, \hat{\beta}_5) \\ + 2u_1^2 u_2^2 \text{ cov } (\hat{\beta}_3, \hat{\beta}_5)] du_1\, du_2 - \int_{-a_{i-1}}^{a_{i-1}}\int_{-a_{i-1}}^{a_{i-1}} [\text{var } \hat{\beta}_0 + u_1^2 \text{ var } \hat{\beta}_1 \\ + u_2^2 \text{ var } \hat{\beta}_2 + u_1^4 \text{ var } \hat{\beta}_3 + u_1^2 u_2^2 \text{ var } \hat{\beta}_4 + u_2^4 \text{ var } \hat{\beta}_5 + 2u_1^2 \text{ cov } (\hat{\beta}_0, \hat{\beta}_3) \\ + 2u_2^2 \text{ cov } (\hat{\beta}_0, \hat{\beta}_5) + 2u_1^2 u_2^2 \text{ cov } (\hat{\beta}_3, \hat{\beta}_5)] du_1\, du_2\}.\end{aligned}$$

For the sake of simplicity let

$$A = \text{var } \hat{\beta}_o$$

$$B = \text{cov } (\hat{\beta}_o, \hat{\beta}_3) = \text{cov } (\hat{\beta}_o, \hat{\beta}_5)$$

$$C = \text{var } \hat{\beta}_1 = \text{var } \hat{\beta}_2$$

$$D = \text{var } \hat{\beta}_3 = \text{var } \hat{\beta}_5$$

$$E = \text{cov } (\hat{\beta}_3, \hat{\beta}_5)$$

$$F = \text{var } \hat{\beta}_4 .$$

Thus

$$\text{ave var } \hat{y}(u_1, u_2) = \sum_{i=1}^{n} K_i \{ [2Aa_i u_2 + (2/3)(2B + C)(a_i^3 u_2 + a_i u_2^3)$$

$$+ (2/5)\ D\ (a_i^5 u_2 + a_i u_2^5) + (4/9)(2E + F)\ a_i^3 u_2^3\ ] \Big|_{u_2 = -a_i}^{u_2 = a_i}$$

$$-[2Aa_i u_2 + (2/3)(2B + C)(a_i^3 u_2 + u_1 u_2^3) + (2/5)\ D\ (a_i^5 u_2 + a_i u_2^5)$$

$$+ (4/9)(2E + F)\ a_i^3 u_2^3] \Big|_{u_2 = -a_{i-1}}^{u_2 = a_{i-1}} \}$$

$$= \sum_{i=1}^{n} \frac{M_i}{4(a_i^2 - a_{i-1}^2)} \{4Aa_i^2 + (8/3)(2B + C)a_i^4 + [(8/5)\ D + (4/9)(2E + F)]a_i^6$$

$$-[4Aa_{i-1}^2 + (8/3)(2B + C)\ a_i^4 + [(8/5)\ D + (4/9)(2E + F)]a_{i-1}^6]\}$$

$$= \sum_{i=1}^{n} M_i \{A + (2/3)(2B + C)(a_i^2 + a_{i-1}^2) + ((2/5)\ D + (1/9)(2E + F))(a_i^4$$

$$+ a_i^2 a_{i-1}^2 + a_{i-1}^4)\}$$

$$\text{ave var } \hat{y}(u_1, u_2) = \text{var } \hat{\beta}_o + \sum_{i=1}^{n} M_i \{(1/3)(4 \text{ cov } (\hat{\beta}_o, \hat{\beta}_3)$$

$$+ \text{var } \hat{\beta}_1 + \text{var } \hat{\beta}_2)(a_i^2 + a_{i-1}^2) + [(1/5)(\text{var } \hat{\beta}_3 + \text{var } \hat{\beta}_5)$$

$$+ (1/9)(2 \text{ cov } (\hat{\beta}_3, \hat{\beta}_5) + \text{var } \hat{\beta}_4)](a_i^4 + a_i^2 a_{i-1}^2 + a_{i-1}^4)\}.$$

This completes the proof.

Theorem 5.2 If the total probability mass $M = 1$ is assigned to the n subregions

$$R_i = [(u_1, u_2) \mid a_{i-1}^2 \leq u_1^2 + u_2^2 \leq a_i^2],$$

$(i = 1, 2, \ldots, n;\ a_o = 0)$, of the region R_c, then the average variance of $\hat{y}(u_1, u_2)$ over R_c is given by

$$\begin{aligned} \text{ave var } \hat{y}(u_1, u_2) &= \text{var } \hat{\beta}_0 + (1/2)(2 \text{ cov } (\hat{\beta}_o, \hat{\beta}_3) + \text{var } \hat{\beta}_1)\cdot \\ &\sum_{i=1}^{n} M_i(a_i^2 + a_{i-1}^2) + (1/24)(6 \text{ var } \hat{\beta}_3 + 2 \text{ cov } (\hat{\beta}_3, \hat{\beta}_5) \\ &+ \text{var } \hat{\beta}_4) \sum_{i=1}^{n} M_i(a_i^4 + a_i^2 a_{i-1}^2 + a_{i-1}^4) \end{aligned}$$

where M_i denotes the probability mass assigned to R_i and $\sum_{i=1}^{n} M_i = 1$.

Proof: Let

$$A_i = \pi(a_i^2 - a_{i-1}^2)$$

be the area of R_i, then $f_i(u_1, u_2) = K_i$,

where

$$\begin{aligned} K_i &= M_i/A_i \text{ if } (u_1, u_2) \in R_i \\ &= 0 \qquad \text{otherwise} \end{aligned}$$

is the density function of (u_1, u_2) in R_c. Thus

$$\begin{aligned} \text{ave var } \hat{y}(u_1, u_2) &= \sum_{i=1}^{n} 4\Big[\int_o^{a_i}\int_o^{\sqrt{a_i^2 - u_2^2}} f_i(u_1, u_2) \text{ var } \hat{y}(u_1, u_2) du_1\, du_2 \\ &- \int_o^{a_i}\int_o^{\sqrt{a_{i-1}^2 - u_2^2}} f_i(u_1, u_2) \text{ var } \hat{y}(u_1, u_2) du_1\, du_2\Big] \end{aligned}$$

$$\begin{aligned} = \sum_{i=1}^{n} 4K_i\Big\{\int_o^{a_i}\int_o^{\sqrt{a_i^2 - u_2^2}} &[\text{var } \hat{\beta}_0 + u_1^2 \text{ var } \hat{\beta}_1 + u_2^2 \text{ var } \hat{\beta}_2 + u_1^4 \text{ var } \hat{\beta}_3 \\ &+ u_1^2 u_2^2 \text{ var } \hat{\beta}_4 + u_2^4 \text{ var } \hat{\beta}_5 + 2u_1^2 \text{ cov } (\hat{\beta}_o, \hat{\beta}_3) + 2u_2^2 \text{ cov } (\hat{\beta}_o, \hat{\beta}_5) \end{aligned}$$

$$+ 2u_1^2u_2^2 \text{ cov } (\hat{\beta}_3, \hat{\beta}_5)]du_1\, du_2 - \int_o^{a_i}\int^{\sqrt{a_{i-1}^2 - u_2^2}} [\text{var } \hat{\beta}_o + u_1^2 \text{ var } \hat{\beta}_1$$

$$+ u_2^2 \text{ var } \hat{\beta}_2 + u_1^4 \text{ var } \hat{\beta}_3 + u_1^2u_2^2 \text{ var } \hat{\beta}_4 + u_2^4 \text{ var } \hat{\beta}_5 + 2u_1^2 \text{ cov } (\hat{\beta}_o, \hat{\beta}_3)$$

$$+ 2u_2^2 \text{ cov } (\hat{\beta}_o, \hat{\beta}_5) + 2u_1^2u_2^2 \text{ cov } (\hat{\beta}_3, \hat{\beta}_5)]du_1\, du_2\} .$$

Let A, B, C, D, E, F denote the same quantities as in Theorem 5.1 and make the following transformation to polar coordinates. Let

$$u_1 = r \cos \theta$$

$$u_2 = r \sin \theta, \text{ then}$$

$$J = \begin{vmatrix} \partial u_1/\partial r & \partial u_1/\partial\theta \\ \partial u_2/\partial r & \partial u_2/\partial\theta \end{vmatrix} = \begin{vmatrix} \cos \theta & - r \sin \theta \\ \sin \theta & r \cos \theta \end{vmatrix} = r .$$

Then we have

$$\text{ave var } \hat{y}(u_1, u_2) = \sum_{i=1}^{n} K_i\{\int_o^{2\pi}\int_{a_{i-1}}^{a_i} [A + (2B + C)r^2 + Dr^4(\cos^4\theta + \sin^4\theta)$$

$$+ (2E + F)\, r^4 \cos^2\theta \sin^2\theta]\, r\, dr\, d\theta\}$$

$$= \sum_{i=1}^{n} [M_i/\pi(a_i^2 - a_{i-1}^2)](\pi)\{A(a_i^2 - a_{i-1}^2) + (1/2)(2B + C)(a_i^4 - a_{i-1}^4)$$

$$+ (1/24)(a_i^6 - a_{i-1}^6)(6D + 2E + F)\}$$

$$= A + (1/2)(2B + C) \sum_{i=1}^{n} M_i(a_i^2 + a_{i-1}^2) + (1/24)(6D + 2E + F)\cdot$$

$$\sum_{i=1}^{n} M_i(a_i^4 + a_i^2a_{i-1}^2 + a_{i-1}^4)$$

$$\text{ave var } \hat{y}(u_1, u_2) = \text{var } \hat{\beta}_o + (1/2)[2 \text{ cov } (\hat{\beta}_o, \hat{\beta}_3)$$

$$+ \text{var } \hat{\beta}_1] \sum_{i=1}^{n} M_i(a_i^2 + a_{i-1}^2) + (1/24)(6 \text{ var } \hat{\beta}_3 + 2 \text{ cov } (\hat{\beta}_3, \hat{\beta}_5)$$

$$+ \text{var } \hat{\beta}_4) \sum_{i=1}^{n} M_i(a_i^4 + a_i^2a_{i-1}^2 + a_{i-1}^4).$$

This completes the proof.

5.2 Designs Which Have Minimum Ave Var $\hat{y}(u_1, u_2)$ in R and R_c

The symmetrical designs which have the minimum ave var $\hat{y}(u_1, u_2)$ in R and R_c with $a_1 = 1$, $a_o = 0$ and $M_1 = 1$ were determined for N = 8, 9, 12, 13, P = 5, 7, ..., 49 and N = 12, P = 4, 6, ..., 50. There are too many for the space available here; therefore the optimal designs for which N = 8, 9, 12, 13, P = 5, 7, 9, ∞ and N = 12, P = 4, 6, 8, ∞, were chosen to be exhibited in Tables VII and VIII.

To obtain the optimal designs for a fixed N as $P \rightarrow \infty$, we need the following theorems.

5.3 Minimum Average Variance Designs in R as $P \rightarrow \infty$

Theorem 5.3 If N = 8, P is odd and if the limiting points are (1, 1), (1, -1), (-1, 1), (-1, -1), (M, 0), (0, M), (-M, 0), (0, -M), then the design which has the minimum average variance of $\hat{y}(u_1, u_2)$ in R occurs at M = 0.80401 as $P \rightarrow \infty$.

Proof: If we use the above points, the

$$\text{ave var } \hat{y}(u_1, u_2) = (4 + M^4)/4(2 - M^2) + (2/3)[-(2 + M^2)/2(2 - M^2)^2 + 1/(4 + 2M^2)] + (2/5)(4 + 4M^2 + 3M^4)/4M^4(2 - M^2)^2 + (1/9)[(M^4 + 4M^2 - 4)/2M^4(2 - M^2)^2 + 1/4].$$

The value of M which minimizes this equation in [0,1] is M = 0.80401, found by taking the derivative of the above equation and solving for the roots of the derivative in [0,1].

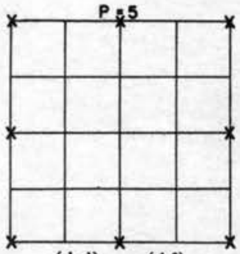
Theorem 5.4 If N = 9, P is odd and if the limiting points are (1, 1), (1, -1), (-1, 1), (-1, -1), (0, 0), (M, 0), (0, M), (-M, 0), (0, -M), then the design which has the minimum ave var $\hat{y}(u_1, u_2)$ in R occurs at M = 0.910001.

TABLE VII

MINIMUM AVE VAR $\hat{y}(u_1,u_2)$ DESIGNS IN R FOR SPECIFIED N AND P^2

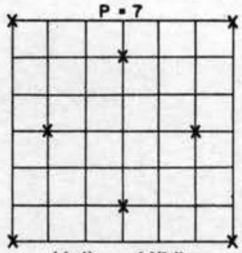
N = 8

P = 5



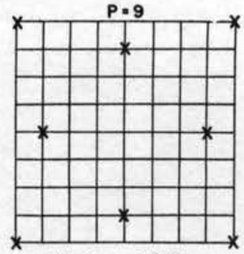
(-1,-1)	(-1,0)
(-1,1)	(0,-1)
(1,-1)	(1,0)
(1,1)	(0,1)

P = 7



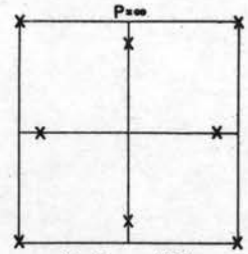
(-1,-1)	(-2/3,0)
(-1,1)	(0,-2/3)
(1,-1)	(2/3,0)
(1,1)	(0,2/3)

P = 9



(-1,-1)	(-3/4,0)
(-1,1)	(0,-3/4)
(1,-1)	(3/4,0)
(1,1)	(0,3/4)

P = ∞

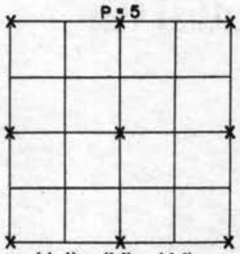


(-1,-1)	(-M,0)
(-1,1)	(0,-M)
(1,-1)	(M,0)
(1,1)	(0,M)

M = 0.80401

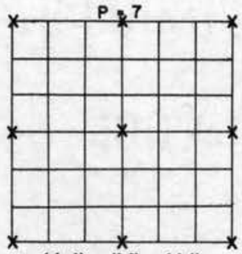
N = 9

P = 5



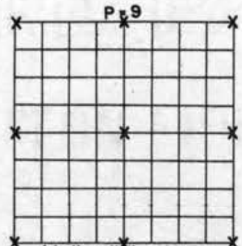
(-1,-1)	(0,0)	(-1,0)
(-1,1)		(0,-1)
(1,-1)		(1,0)
(1,1)		(0,1)

P = 7



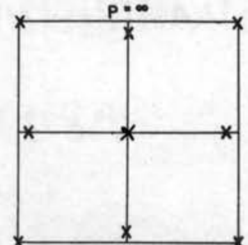
(-1,-1)	(0,0)	(-1,0)
(-1,1)		(0,-1)
(1,-1)		(1,0)
(1,1)		(0,1)

P = 9



(-1,-1)	(0,0)	(-1,0)
(-1,1)		(0,-1)
(1,-1)		(1,0)
(1,1)		(0,1)

P = ∞

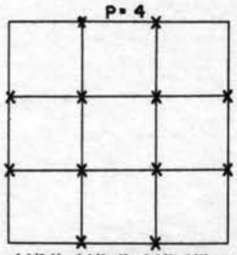


(-1,-1)	(0,0)	(-M,0)
(-1,1)		(0,-M)
(1,-1)		(M,0)
(1,1)		(0,M)

M = 0.910001

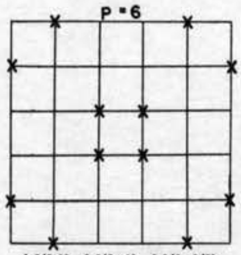
N = 12

P = 4



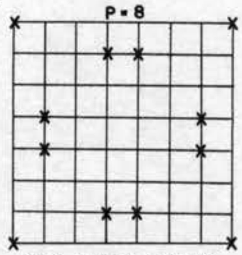
(-1/3,1)	(-1/3,-1)	(-1/3,-1/3)
(1,-1/3)	(-1,-1/3)	(-1/3,1/3)
(1/3,1)	(1/3,-1)	(1/3,-1/3)
(1,1/3)	(-1,1/3)	(1/3,1/3)

P = 6



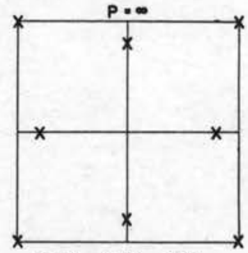
(-3/5,1)	(-3/5,-1)	(-1/5,-1/5)
(1,-3/5)	(-1,-3/5)	(-1/5,1/5)
(3/5,1)	(3/5,-1)	(1/5,-1/5)
(1,3/5)	(-1,3/5)	(1/5,1/5)

P = 8



(-1,-1)	(-1/7,5/7)	(-1/7,-5/7)
(-1,1)	(5/7,-1/7)	(-5/7,-1/7)
(1,-1)	(1/7,5/7)	(1/7,-5/7)
(1,1)	(5/7,1/7)	(-5/7,1/7)

P = ∞

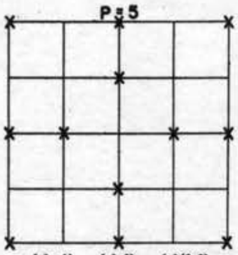


(-1,-1)	(-M,0)	(0,-M)
(-1,1)	(-M,0)	(0,-M)
(1,-1)	(M,0)	(0,M)
(1,1)	(M,0)	(0,M)

M = 0.8033

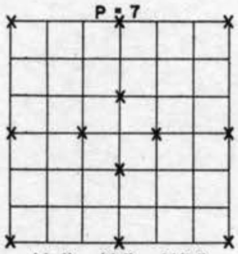
N = 12

P = 5



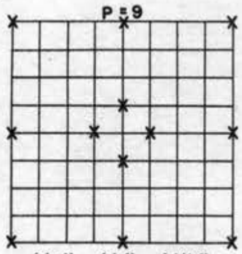
(-1,-1)	(-1,0)	(-1/2,0)
(-1,1)	(0,-1)	(0,-1/2)
(1,-1)	(1,0)	(1/2,0)
(1,1)	(0,1)	(0,-1/2)

P = 7



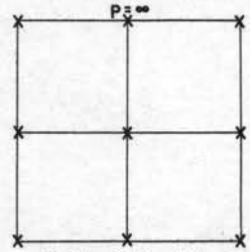
(-1,-1)	(-1,0)	(-1/3,0)
(-1,1)	(0,-1)	(0,-1/3)
(1,-1)	(1,0)	(1/3,0)
(1,1)	(0,1)	(0,1/3)

P = 9



(-1,-1)	(-1,0)	(-1/4,0)
(-1,1)	(0,-1)	(0,-1/4)
(1,-1)	(1,0)	(1/4,0)
(1,1)	(0,1)	(0,1/4)

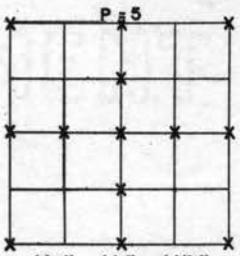
P = ∞



(-1,-1)	(0,-1)	(0,0)
(-1,1)	(-1,0)	(0,0)
(1,-1)	(0,1)	(0,0)
(1,1)	(1,0)	(0,0)

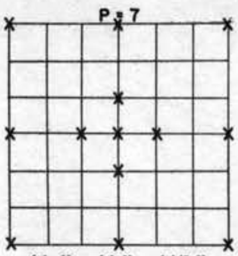
N = 13

P = 5



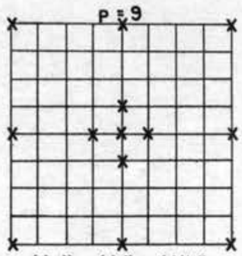
(-1,-1)	(-1,0)	(-1/2,0)
(-1,1)	(0,-1)	(0,-1/2)
(1,-1)	(1,0)	(1/2,0)
(1,1)	(0,1)	(0,-1/2)
	(0,0)	

P = 7



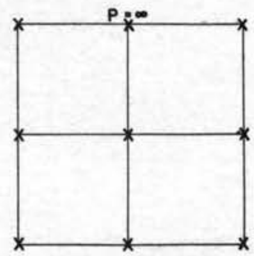
(-1,-1)	(-1,0)	(-1/3,0)
(-1,1)	(0,-1)	(0,-1/3)
(1,-1)	(1,0)	(1/3,0)
(1,1)	(0,1)	(0,1/3)
	(0,0)	

P = 9



(-1,-1)	(-1,0)	(-1/4,0)
(-1,1)	(0,-1)	(0,-1/4)
(1,-1)	(1,0)	(1/4,0)
(1,1)	(0,1)	(0,1/4)
	(0,0)	

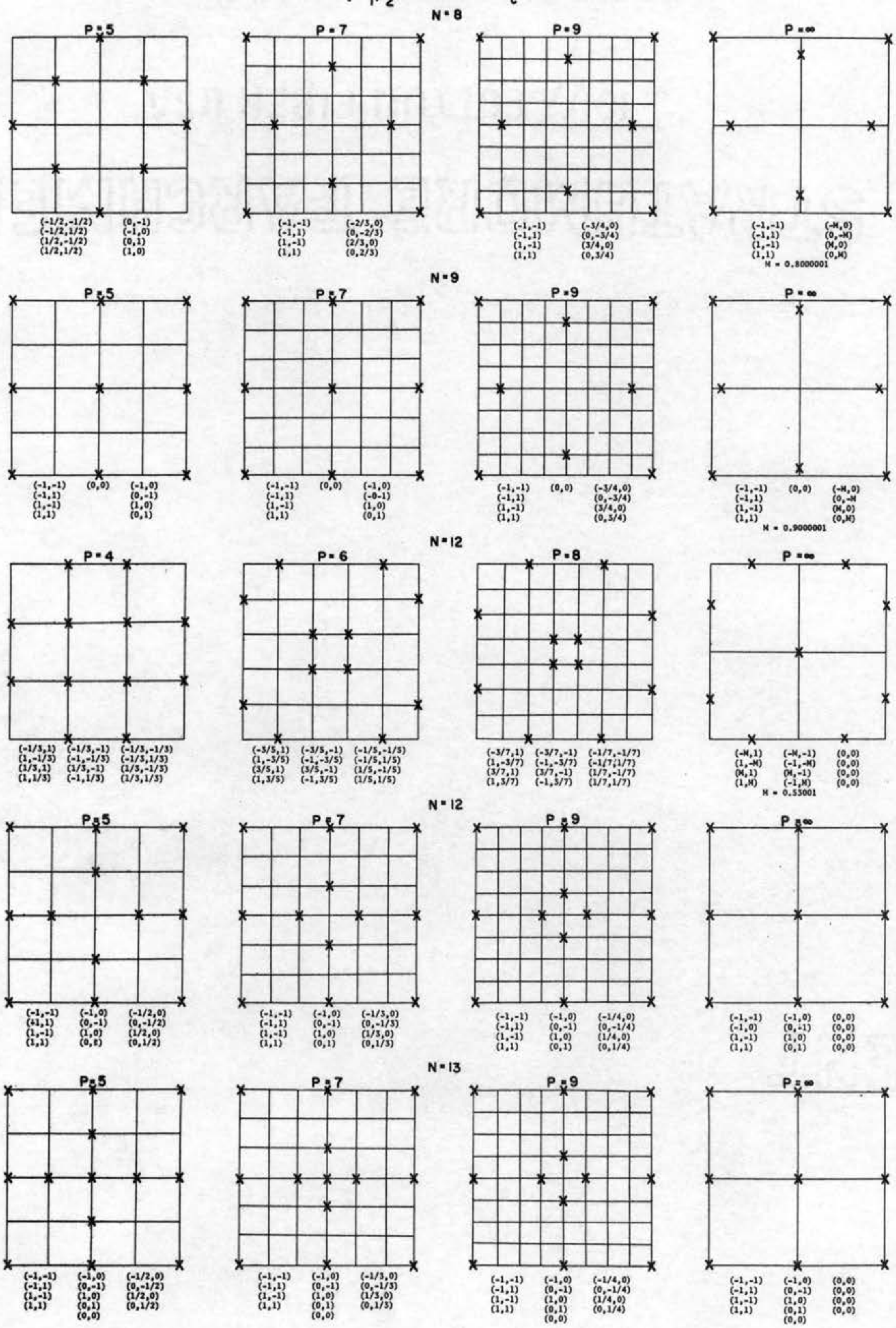
P = ∞



(-1,-1)	(-1,0)	(0,0)
(-1,1)	(0,-1)	(0,0)
(1,-1)	(1,0)	(0,0)
(1,1)	(0,2)	(0,0)
	(0,0)	

TABLE VIII

MINIMUM AVE VAR $\hat{y}(u_1,u_2)$ DESIGNS IN R_c FOR SPECIFIED N AND P^2



Proof: The proof is similar to that for Theorem 5.3.

Theorem 5.5 If $N = 12$, P is even and if the limiting points are $(1, 1)$, $(1, -1)$, $(-1, 1)$, $(-1, -1)$, $(M, 0)$, $(M, 0)$, $(0, M)$, $(0, M)$, $(-M, 0)$, $(-M, 0)$, $(0, -M)$, $(0, -M)$, then the design which has the minimum ave var $\hat{y}(u_1, u_2)$ in R occurs at $M = .8033$ as $P \to \infty$.

Proof: The proof is similar to that for Theorem 5.3.

Theorem 5.6 If $N = 12$, P is odd and if the limiting points are $(1, 1)$, $(1, -1)$, $(-1, 1)$, $(-1, -1)$, $(1, 0)$, $(0, 1)$, $(-1, 0)$, $(0, -1)$ $(M, 0)$, $(0, M)$, $(M, 0)$, $(0, M)$, then the design which has the minimum ave var $\hat{y}(u_1, u_2)$ in R occurs at $M = 0$ as $P \to \infty$.

Proof: The proof is similar to the proof of Theorem 5.3.

Theorem 5.7 If $N = 13$, P is odd and if the limiting points are $(1, 1)$, $(1, -1)$, $(-1, 1)$, $(-1, -1)$, $(1, 0)$, $(0, 1)$, $(-1, 0)$, $(0, -1)$, $(0, 0)$, $(M, 0)$, $(0, M)$, $(-M, 0)$, $(0, -M)$, then the design which has the minimum ave var $\hat{y}(u_1, u_2)$ in R occurs at $M = 0$ as $P \to \infty$.

Proof: The proof is similar to the proof of Theorem 5.3.

5.4 Minimum Average Variance Designs in R_c as $P \to \infty$

Theorem 5.8 If $N = 8$, P is odd and if the limiting points are $(1, 1)$, $(1, -1)$, $(-1, 1)$, $(-1, -1)$, $(M, 0)$, $(0, M)$, $(-M, 0)$, $(0, -M)$, then the design which has the minimum ave var $\hat{y}(u_1, u_2)$ is R_c occurs at $M = .8000001$ as $P \to \infty$.

Proof: If we use the above points, the

$$\text{ave var } \hat{y}(u_1, u_2) = (4 + M^4)/4(2 - M^2)^2 + (1/2)[-(2 + M^2)/2(2 - M^2)^2 + 1/2(2 + M^2)] + (1/24)[3(4 + M^2 + 3M^4)/2M^4(2 - M^2)^2 + (M^4 + 4M^2 - 4)/2M^4(2 - M^2)^2 + 1/4].$$

The value of M which minimizes this equation in [0,1] is M = 0.8000001, found by taking the derivative of the above equation and solving for the roots of the derivative in [0,1].

Theorem 5.9 If N = 9, P is odd and if the limiting points are (1, 1), (1, -1), (-1, 1), (-1, -1), (0, 0), (M, 0), (0, M), (-M, 0), (0, -M), then the design which has the minimum ave var $\hat{y}(u_1, u_2)$ in R_c occurs at M = 0.9000001 as $P \rightarrow \infty$.

Proof: The proof is similar to the proof of Theorem 5.8.

Theorem 5.10 If N = 12, P is even and if the limiting points are (1, M), (M, 1), (1, -M), (-M, 1), (-1, M), (M, -1), (-1, -M), (-M, -1), (0, 0), (0, 0), (0, 0), (0, 0), then the design which has the minimum ave var $\hat{y}(u_1, u_2)$ in R_c occurs at M = 0.53001 as $P \rightarrow \infty$.

Proof: The proof is similar to that for Theorem 5.8.

Theorem 5.11 If N = 12, P is odd and if the limiting points are (1, 1), (1, -1), (-1, 1), (-1, -1,), (1, 0), (0, 1), (-1, 0), (0, -1), (M, 0), (0, M), (-M, 0), (0, -M), then the design which has the minimum ave var $\hat{y}(u_1, u_2)$ in R_c occurs at M = 0 as $P \rightarrow \infty$.

Proof: The proof is similar to that for Theorem 5.8.

Theorem 5.12 If $N = 13$, P is odd and if the limiting points are $(1, 1)$, $(1, -1)$, $(-1, 1)$, $(-1, -1)$, $(1, 0)$, $(0, 1)$, $(-1, 0)$, $(0, -1)$, $(0, 0)$, $(M, 0)$, $(0, M)$, $(-M, 0)$, $(0, -M)$, then the design which has the minimum ave var $\hat{y}(u_1, u_2)$ in R_c occurs at $M = 0$ as $P \rightarrow \infty$.

Proof: The proof is similar to that for Theorem 5.8

The value of M for which we have been solving in the preceding Theorems is related to the partitions of the region $-1 \leq x_i \leq 1$. In fact, $M = (P + 1 - 2i)/(P - 1)$ where i is the number of partitions from the boundary of the region.

The design which has the min ave var $\hat{y}(u_1, u_2)$ in R are very similar to those for R_c and most closely resemble the minimax characteristic root designs.

To illustrate which of these optimality criteria should be used in an experiment, consider the following examples.

Example 5.1: Suppose an experimenter has two factors, each with only five levels at which measurements can be made, and he can only afford nine observations. The experimenter should choose an optimality criterion depending upon his preference, then use the points indicated for the optimal design with $N = 9$ and $P = 5$.

Example 5.2: Suppose an experimenter has two factors which can be measured at very small intervals. After choosing the optimality criterion desired, he could use the limiting design to specify the values for the N points which he could afford.

CHAPTER VI

SUMMARY AND EXTENSIONS

In this thesis symmetrical experimental designs based on the expansion of P^n as $(\sum_{i=1}^{k} p_i)^n$ were defined and studied. For a given number of design points, N, and a specified P^2, there exists a class C of symmetrical designs. The designs in C were compared to determine which was optimal using specified optimality criteria and assuming the model

$$y(x_1, x_2) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1^2 + \beta_4 x_1 x_2 + \beta_5 x_2^2 + \epsilon.$$

In Chapter II the procedure for determining symmetrical designs and the optimality criteria by which these designs were compared was defined and discussed. Thomas (7) developed the method of expressing P^n as $(\sum_{i=1}^{k} p_i)^n$, but his investigation was oriented toward fractional replication and analysis of variance methods. The designs obtained in this study are best used in determining the shape of a response surface in a specified region.

Gillett (3) compared experimental designs using some of the criteria used here. However his discussion involved primarily designs with only three design points and assuming a linear model. Chapters IV and V were devoted to the problem of determining the $\min_D \max_{\hat{\beta}} \text{var } \hat{\beta}$ design, $\min_D$ generalized var $\hat{\beta}$ design, $\min_D \max_r$ characteristic root of

$(X'X)^{-1}$ design, and min ave var $\hat{y}(u_1, u_2)$ design in R and R_c, and these designs for specified N and P^2 are exhibited in Tables IV, V, VI, VII and VIII.

The method of obtaining symmetrical designs from P^n factorials where the design points will be chosen according to the rule for symmetry which is a generalization of the "rule" defined for the P^2 case in Chapter II will be discussed briefly now. The "points" of a design will be used to estimate the coefficients, β_j, of the quadratic model

$$y(x_1, x_2, \ldots, x_n) = \beta_0 x_0 + \sum_{i=1}^{n} \beta_i x_i + \sum_{j=n+1}^{n(n+3)/2} \beta_j f_j(x_k, x_t) + \epsilon$$

where $-1 \leq x_i \leq$, $i = 1, 2, \ldots, n$, $x_0 = 1$, $\epsilon \sim N(0, \sigma^2)$ and $f_j(x_k, x_t) = x_k x_t$ for all $k, t = 1, 2, \ldots, n$ and $k \leq t$.

First, it is necessary to extend the rule for symmetry to any P^n. From Chapter I we find that a P^n factorial may be expressed as $(\sum_{i=1}^{k} p_i)^n$. We require that $p_i = 2$, $i = 1, 2, \ldots, k - 1$, and $p_k = 1$ if P is odd or $p_k = 2$ if P is even. The φ_i should be partitioned as follows: $\varphi_1 = (1,P)$, $\varphi_2 = (2,P-1)$, $\ldots$, $\varphi_k = (P/2, (P+2)/2)$ if P is even or $\varphi_k = ((P-1)/2)$ if P is odd. We can now write $(\sum_{i=1}^{k} p_i)^n$ as $(\sum_{i=1}^{(P-1)/2} 2_i + 1)^n$ for odd P and $(\sum_{i=1}^{P/2} 2_i)^n$ for even P. To determine all the possible reduced symmetrical designs for a specified P^n, we need only to expand

$$(\sum_{i=1}^{k} p_i)^n = \sum_{n_1=0}^{n} \sum_{n_2=0}^{n} \cdots \sum_{n_k=0}^{n} [n!/(n_1!n_2! \ldots n_k!)] p_1^{n_1} p_2^{n_2} \cdots p_k^{n_k}.$$

Each term of this expansion represents a reduced symmetrical design.

Example 6.1: Consider a P^n factorial where $P = 5$ and $n = 3$, Thus 5^3 may be expressed as

$$5^3 = (2_1 + 2_2 + 1)^3 = 2_1^3 + 2_2^3 + 1^3 + 3\,(2_1 x 2_2^2) + 3\,(2_1 x 1^2)$$

$$+ 3\,(2_2 x 1^2) + 3\,(2_1^2 x 2_2) + 3\,(2_1^2 x 1) + 3\,(2_2^2 x 1) + 6\,(2_1 x 2_2 x 1).$$

Thus there are 10 reduced symmetrical designs for a 5^3. If we denote the 5 levels with the numerals 1, 2, 3, 4, 5, then φ_i may be partitioned as $\varphi_1 = (1,5)$, $\varphi_2 = (2,4)$, and $\varphi_3 = (3)$. Then the points of the reduced design obtained from the term $3(2_1^2 x 1)$ are (1,1,3), (1,5,3), (5,1,3,), (5,5,3), (1,3,1), (1,3,5), (5,3,1), (5,3,5), (3,1,1), (3,1,5), (3,5,1), (3,5,5).

All possible symmetrical designs can now be obtained by taking all combinations of reduced symmetrical designs.

There are several possible extensions of this study. Optimal designs for P^n with $n > 2$ were not examined here because as n increases the number of symmetrical designs available for a particular N becomes very large and computing facilities were not available to make this study. Designs which have a minimum average variance $\hat{y}(u_1, u_2)$ in R and R_c could be studied with two or more subregions and different distributions of the total probability mass. Also the symmetrical designs obtained here could be studied from an analysis of variance viewpoint.

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